

Two-particle model with noncommuting operators of coordinates and momenta

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Abstract

A nonrelativistic equation for the system of two interacting particles within the framework of a model with noncommuting operators of coordinates and momenta of different particles is proposed, and a self-consistent system of equations for the wave function of every quantum state is deduced. Solutions for the lowest states of a hydrogenlike atom are found, and the comparison with analogous solutions of the Klein-Gordon equation for the relativistic spinless problem is performed. In the case where the size of a two-particle system and the Compton wavelengths of particles forming it are of the same order, the essential differences with solutions of the Schrödinger nonrelativistic equation are revealed.

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I. INTRODUCTION

For a system of two interacting particles, the well-known Schrödinger equation [1] can be derived through the formal substitution of the quantities E , \mathbf{r}_1 , \mathbf{r}_2 , \mathbf{p}_1 , and \mathbf{p}_2 by the relevant operators [2] on both sides of the relation $E = H(\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2)$, where H is the classical Hamilton function of a system of two interacting particles. Here, \mathbf{r}_1 and \mathbf{r}_2 are Cartesian coordinates of two particles with momenta \mathbf{p}_1 and \mathbf{p}_2 , respectively.

The operators $\hat{\mathbf{r}}_1$, $\hat{\mathbf{r}}_2$, $\hat{\mathbf{p}}_1$, and $\hat{\mathbf{p}}_2$ are such that they satisfy the following commutation relations:

$$[\hat{x}_k, \hat{p}_{kx}] = [\hat{y}_k, \hat{p}_{ky}] = [\hat{z}_k, \hat{p}_{kz}] = i\hbar \quad (k = 1, 2). \quad (1)$$

Here, $\hbar = h/2\pi$, where h is the universal constant introduced by Planck. All other possible commutation relations equal zero, including

$$[\hat{x}_k, \hat{p}_{lx}] = [\hat{y}_k, \hat{p}_{ly}] = [\hat{z}_k, \hat{p}_{lz}] = 0 \quad (k \neq l). \quad (2)$$

Equalities (2) are based on the assumption that measurements of coordinates and momenta of different particles do not disturb one another in principle even in the presence of some forces between particles [3]. That is, one supposes that the change in the force action of a particle on another one, caused by a measurement of the coordinate of the first, propagates with finite velocity.

Thus, to derive the Schrödinger nonrelativistic equation for a two-particle system, one uses, on the one hand, the Hamilton classical nonrelativistic function and, on the other hand, the implicit assumption about finiteness of the interaction propagation velocity.

In the fully nonrelativistic quantum theory, we must consider the interaction propagation velocity as infinitely large, which forces us to drop the requirement for the commutation relations (2) to hold. Having accepted this viewpoint, we will consider that, under a measurement of the coordinate of the first particle, there occurs the uncontrolled transfer of momentum not only to this particle but to the whole system since the particles are connected through the interaction potential, whose propagation velocity is infinitely large.

Therefore, it is natural to require that the commutator of the coordinate operator of any particle and the of operator total momentum of the system $\hat{\mathbf{P}}_c = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2$ be equal to $i\hbar$:

$$[\hat{x}_k, \hat{P}_{cx}] = [\hat{y}_k, \hat{P}_{cy}] = [\hat{z}_k, \hat{P}_{cz}] = i\hbar \quad (k = 1, 2). \quad (3)$$

Note that relations (3) hold true also for a Schrödinger nonrelativistic equation. Namely, they allow one to construct the operator of coordinates of the center of mass of the system, whose commutator with the operator of total momentum equals $i\hbar$. On the contrary, the fulfillment of relations (1) is not obligatory for a system of interacting particles, and we intend to reject this requirement.

The first attempt to construct the nonrelativistic equation for a system of interacting particles in the framework of the model with noncommuting operators of coordinates and momenta of different particles was undertaken in [4,5]. However, the theory proposed there is phenomenological, i.e., it contains a parameter whose determination is ambiguous. Moreover, the proposed self-consistent system of integro-differential equations was faced with difficulties of the probabilistic interpretation of a wave function. The present work is devoted to the elimination of the drawbacks mentioned above.

II. FULLY NONRELATIVISTIC STATEMENT OF THE QUANTUM TWO-BODY PROBLEM

The probabilistic interpretation of the square of the modulus of a wave function is possible only under the assumption that measurements of coordinates or momenta of various particles do not principally disturb one another even if there exists some interaction between particles [3]. This means that the operators of coordinates and momenta of two particles commute with each other.

As noted above, the operators of coordinates and momenta of different particles do not commute with one another in the general case. Let

$$[\hat{x}_1, \hat{p}_{2x}] = i\hbar \hat{f}_1, \quad (4)$$

where \hat{f}_1 is a dimensionless Hermitian operator. Then it follows from Eq. (3) that

$$[\hat{x}_1, \hat{p}_{1x}] = i\hbar(1 - \hat{f}_1). \quad (5)$$

By analogy, if

$$[\hat{x}_2, \hat{p}_{1x}] = i\hbar \hat{f}_2, \quad (6)$$

then

$$[\hat{x}_2, \hat{p}_{2x}] = i\hbar(1 - \hat{f}_2). \quad (7)$$

The dimensionless Hermitian operators \hat{f}_1 and \hat{f}_2 depend generally on the interaction force between particles \mathbf{F}_{12} and on the masses of interacting particles m_1 and m_2 . The operators \hat{f}_1 and \hat{f}_2 cannot depend on a direction of the vector \mathbf{F}_{12} , since the commutation relations for the x , y , and z components should be identical analogously to (4)-(7), since there are no separated directions in the system, and the independent variables in the Cartesian coordinate system are fully equivalent. For this reason, the operators \hat{f}_1 and \hat{f}_2 are only functions of the absolute value of a force, i.e., of $|\mathbf{F}_{12}|$:

$$\hat{f}_1 \equiv \hat{f}_1(m_1, m_2, |\mathbf{F}_{12}|), \quad \hat{f}_2 \equiv \hat{f}_2(m_1, m_2, |\mathbf{F}_{12}|). \quad (8)$$

Let us make permutation of m_1 and m_2 . Then

$$[\hat{x}_1, \hat{p}_{2x}] = i\hbar \hat{f}_1(m_2, m_1, |\mathbf{F}_{12}|), \quad [\hat{x}_2, \hat{p}_{1x}] = i\hbar \hat{f}_2(m_2, m_1, |\mathbf{F}_{12}|). \quad (9)$$

Compare (9) with (4), (6). Considering that the physical situation has not changed, we get

$$\hat{f}_1(m_2, m_1, |\mathbf{F}_{12}|) = \hat{f}_2(m_1, m_2, |\mathbf{F}_{12}|). \quad (10)$$

Thus, we have one unknown operator $\hat{f}_1(m_1, m_2, |\mathbf{F}_{12}|)$. For $m_2 \rightarrow 0$, \hat{f}_1 must tend to zero since, in the absence of the second particle, the whole momentum transferred under the measurement of the coordinate x_1 falls to the first one. If $|\mathbf{F}_{12}| \rightarrow 0$, then $\hat{f}_1 \rightarrow 0$, i.e., without any interaction forces between particles, the operators of coordinates and momenta of different particles commute among themselves. The situation $|\mathbf{F}_{12}| \rightarrow \infty$ corresponds to the case where we have one particle of mass M formed by two strongly bound particles

with masses m_1 and m_2 . Therefore, the momentum, received under a measurement of some coordinate, is distributed proportionally to masses of particles. This enables us to write down \hat{f}_1 as $\hat{f}_1 = m_2/M$. Here, $M = m_1 + m_2$ is the system mass.

Therefore, without loss of generality, we can present the operator \hat{f}_1 as

$$\hat{f}_1 = \frac{m_2}{M} \hat{\varepsilon}(|\mathbf{F}_{12}|, m_1, m_2), \quad (11)$$

where $\hat{\varepsilon}$ is a new operator, which is assumed to be symmetric with respect to the masses of particles m_1 and m_2 . In what follows, we will omit its explicit dependence on masses to shorten formulas, namely, $\hat{\varepsilon}(|\mathbf{F}_{12}|, m_1, m_2) \equiv \hat{\varepsilon}(|\mathbf{F}_{12}|)$. For $|\mathbf{F}_{12}| \rightarrow 0$, $\hat{\varepsilon} \rightarrow 0$, and $\hat{\varepsilon} \rightarrow 1$ for $|\mathbf{F}_{12}| \rightarrow \infty$.

For the noncommuting operators \hat{x}_1 and \hat{p}_{2x} , the uncertainty relation has the form

$$\Delta x_1 \Delta p_{2x} \geq \frac{\hbar m_2}{2 M} \left| \frac{\langle \Psi | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right|, \quad (12)$$

where $\langle \Psi | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi \rangle (\langle \Psi | \Psi \rangle)^{-1} \equiv \varepsilon$ is a quantum-mechanical average of the operator $\hat{\varepsilon}$ in the state $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$.

Assume now that the two-particle system has only one quantum state $\Psi_1(\mathbf{r}_1, \mathbf{r}_2, t)$. If we substitute the operator $\hat{\varepsilon}$ in the formula for \hat{f}_1 by its quantum-mechanical average $\langle \Psi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi_1 \rangle (\langle \Psi_1 | \Psi_1 \rangle)^{-1} \equiv \varepsilon_1$, the uncertainty relation (12) does not change. This allows us to construct a nonrelativistic equation for the two-particle system since the operator \hat{f}_1 is constant now.

We present the commutation relations for all operators of coordinates and momenta in the two-body problem (for the y and z components, the commutators are the same) as

$$[\hat{x}_1, \hat{p}_{1x}] = i\hbar \left(1 - \frac{m_2}{M} \varepsilon_1 \right), \quad (13)$$

$$[\hat{x}_2, \hat{p}_{2x}] = i\hbar \left(1 - \frac{m_1}{M} \varepsilon_1 \right), \quad (14)$$

$$[\hat{x}_1, \hat{p}_{2x}] = i\hbar \frac{m_2}{M} \varepsilon_1, \quad (15)$$

$$[\hat{x}_2, \hat{p}_{1x}] = i\hbar \frac{m_1}{M} \varepsilon_1, \quad (16)$$

$$[\hat{x}_1, \hat{x}_2] = 0, \quad (17)$$

$$[\hat{p}_{1x}, \hat{p}_{2x}] = 0. \quad (18)$$

Now we can construct one of the possible representations for the operators of coordinates and momenta of the two-particle system as

$$\hat{\mathbf{r}}_1 = \mathbf{r}_1, \quad (19)$$

$$\hat{\mathbf{r}}_2 = \mathbf{r}_2, \quad (20)$$

$$\hat{\mathbf{p}}_1 = -i\hbar \left(1 - \frac{m_2}{M}\varepsilon_1\right) \nabla_1 - i\hbar \frac{m_1}{M}\varepsilon_1 \nabla_2, \quad (21)$$

$$\hat{\mathbf{p}}_2 = -i\hbar \frac{m_2}{M}\varepsilon_1 \nabla_1 - i\hbar \left(1 - \frac{m_1}{M}\varepsilon_1\right) \nabla_2. \quad (22)$$

Here, as independent variables, we use the coordinates of the particles \mathbf{r}_1 and \mathbf{r}_2 , since the corresponding operators commute with one another.

By changing operators (19)-(22) in the Hamilton function, we get the self-consistent system of integro-differential equations for the nonrelativistic two-body problem:

$$i\hbar \frac{\partial}{\partial t} \Psi_1(\mathbf{r}_1, \mathbf{r}_2, t) = \hat{H} \Psi_1(\mathbf{r}_1, \mathbf{r}_2, t), \quad (23)$$

$$\varepsilon_1 = \frac{\langle \Psi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi_1 \rangle}{\langle \Psi_1 | \Psi_1 \rangle}, \quad (24)$$

where

$$\hat{H} = \hat{T} + \hat{V}(|\mathbf{r}_2 - \mathbf{r}_1|), \quad (25)$$

$$\begin{aligned} \hat{T} = & -\frac{\hbar^2}{2m_1} \left[\left(1 - \frac{m_2}{M}\varepsilon_1\right)^2 + \frac{m_1 m_2}{M^2} \varepsilon_1^2 \right] \Delta_1 - \frac{\hbar^2}{2m_2} \left[\left(1 - \frac{m_1}{M}\varepsilon_1\right)^2 + \frac{m_1 m_2}{M^2} \varepsilon_1^2 \right] \Delta_2 \\ & - \frac{\hbar^2}{2M} [4\varepsilon_1 - 2\varepsilon_1^2] (\nabla_1 \cdot \nabla_2). \end{aligned} \quad (26)$$

We recall that we have received the self-consistent system of equations (23)-(26) for the two-particle system by assuming the existence of only one quantum state $\Psi_1(\mathbf{r}_1, \mathbf{r}_2, t)$.

Under the standard change of variables

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1, \quad (27)$$

$$\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \quad (28)$$

where \mathbf{r} and \mathbf{R} are the relative distance between particles and the coordinates of the center of mass of the system, the system of equations (23)-(26) becomes simpler:

$$i\hbar \frac{\partial}{\partial t} \Psi_1(\mathbf{r}, \mathbf{R}, t) = \left[-\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} - \frac{\hbar^2(1 - \varepsilon_1)^2}{2\mu} \Delta_{\mathbf{r}} + V(r) \right] \Psi_1(\mathbf{r}, \mathbf{R}, t), \quad (29)$$

$$\varepsilon_1 = \frac{\langle \Psi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}(r)|) | \Psi_1 \rangle}{\langle \Psi_1 | \Psi_1 \rangle}. \quad (30)$$

Here, μ is the reduced mass, $\mu = m_1 m_2 / (m_1 + m_2)$. The operator of total momentum reads

$$\hat{\mathbf{P}}_c = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2 = -i\hbar \nabla_{\mathbf{R}}. \quad (31)$$

Let the Hamiltonian H do not explicitly depend on time. Then we obtain, by the substitution

$$\Psi_1 = \psi_1 \exp\left(-i\frac{Et}{\hbar}\right), \quad (32)$$

where ψ_1 depends on coordinates in the configuration space but not on time, the self-consistent system of integro-differential equations for a stationary state of the two-particle system as

$$\left[-\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} - \frac{\hbar^2(1 - \varepsilon_1)^2}{2\mu} \Delta_{\mathbf{r}} + V(r) \right] \psi_1(\mathbf{r}, \mathbf{R}) = E \psi_1(\mathbf{r}, \mathbf{R}), \quad (33)$$

$$\varepsilon_1 = \frac{\langle \psi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}(r)|) | \psi_1 \rangle}{\langle \psi_1 | \psi_1 \rangle}. \quad (34)$$

By the substitution $\psi_1(\mathbf{r}, \mathbf{R}) = \Phi(\mathbf{R}) \varphi_1(\mathbf{r})$, we can separate the motion of the center of mass of the system as a whole. As a result, we arrive at the following self-consistent system of equations:

$$\left[-\frac{\hbar^2(1 - \varepsilon_1)^2}{2\mu} \Delta_{\mathbf{r}} + V(r) \right] \varphi_1(\mathbf{r}) = E_1 \varphi_1(\mathbf{r}), \quad (35)$$

$$\varepsilon_1 = \frac{\langle \varphi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}(r)|) | \varphi_1 \rangle}{\langle \varphi_1 | \varphi_1 \rangle}. \quad (36)$$

As in the Schrödinger nonrelativistic theory, a wave function $\varphi_1(\mathbf{r})$ should be continuous together with its partial derivatives of the first order in the whole space and, in addition, be a bounded single-valued function of its arguments.

As in the Schrödinger theory, for particles interacting by means of a spherically symmetric potential, which depends only on the distance between particles, the wave function $\varphi_1(\mathbf{r})$ can be represented in the following form:

$$\varphi_1(\mathbf{r}) = \frac{1}{r} \chi_{1l}(r) Y_{lm}\left(\frac{\mathbf{r}}{r}\right), \quad (37)$$

where $Y_{lm}(\mathbf{r}/r)$ are orthonormalized spherical functions. Then the function $\chi_{1l}(r)$ satisfies the following system of equations:

$$\left[-\frac{\hbar^2(1 - \varepsilon_{1l})^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) + V(r) \right] \chi_{1l}(r) = E_{1l} \chi_{1l}(r), \quad (38)$$

$$\varepsilon_{1l} = \frac{\langle \chi_{1l} | \hat{\varepsilon}(|\mathbf{F}_{12}(r)|) | \chi_{1l} \rangle}{\langle \chi_{1l} | \chi_{1l} \rangle}. \quad (39)$$

We emphasize that, for a given value of l , the corresponding value of ε_{1l} can exist.

Now we consider the laws of conservation which exist for the proposed fully nonrelativistic scheme of the system of two interacting particles. Since no external fields act on the system, its Hamiltonian must be invariant relative to a parallel translation of the coordinate system in space and time as well as relative to a rotation of the coordinate axes. In addition, the motion equations do not change under a uniform and rectilinear motion of the system (the Galilei invariance).

The Hamiltonian of the isolated system (25) does not depend on time explicitly, and therefore the energy of the system is an integral of motion.

The operator of total momentum of the system $\hat{\mathbf{P}}_c = \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2 = -i\hbar\nabla_1 - i\hbar\nabla_2$ is connected with the operator of infinitesimal translation, which transforms the function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ into the function $\Psi(\mathbf{r}_1 + \delta\mathbf{r}, \mathbf{r}_2 + \delta\mathbf{r})$, by the relation

$$1 + \delta\mathbf{r} \cdot \sum_{k=1}^2 \nabla_k = 1 + \frac{i}{\hbar} \delta\mathbf{r} \cdot \hat{\mathbf{P}}_c \quad (40)$$

and commutes with Hamiltonian (25):

$$[\hat{H}, \hat{\mathbf{P}}_c] = 0, \quad (41)$$

where $\delta\mathbf{r}$ is the vector of infinitesimal parallel displacement of all radius-vectors by the same quantity: $\mathbf{r}_k \rightarrow \mathbf{r}_k + \delta\mathbf{r}$. Thus, three components of the total momentum are integrals of motion, and the total momentum of the two-particle system is conserved.

By virtue of the isotropy of space, the Hamiltonian of a closed system must not vary under a rotation of the whole system by an arbitrary angle around an arbitrary axis. It is sufficient to require the fulfilment of this condition for any infinitesimal rotation, whose vector $\delta\boldsymbol{\Omega}$ is equal to the rotation angle $\delta\Omega$ in modulus and is directed along the rotation axis. The operator of infinitesimal rotation, which transforms the function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ into $\Psi(\mathbf{r}_1 + [\delta\boldsymbol{\Omega} \times \mathbf{r}_1], \mathbf{r}_2 + [\delta\boldsymbol{\Omega} \times \mathbf{r}_2])$, is connected with the operator of total angular momentum of the system through the relation

$$1 + \delta\boldsymbol{\Omega} \cdot \sum_{k=1}^2 [\mathbf{r}_k \times \nabla_k] = 1 + \frac{i}{\hbar} \delta\boldsymbol{\Omega} \cdot \hat{\mathbf{L}} \quad (42)$$

and commutes with Hamiltonian (25) of the system. Thus, the total angular momentum $\hat{\mathbf{L}} = -i\hbar \sum_{k=1}^2 [\mathbf{r}_k \times \nabla_k]$ of the two-particle system is conserved.

It is worth noting the following. If we write the operators $\hat{\mathbf{L}}_1 = [\hat{\mathbf{r}}_1 \times \hat{\mathbf{p}}_1]$ and $\hat{\mathbf{L}}_2 = [\hat{\mathbf{r}}_2 \times \hat{\mathbf{p}}_2]$ in a formal way for each particle, it is easy to show that they and their sum are not angular momenta because they do not satisfy the standard commutation relations peculiar to angular momentum:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y \quad (43)$$

However, from the operators $\hat{\mathbf{r}}_k$ and $\hat{\mathbf{p}}_n$, one can construct the operator possessing the mentioned properties of total angular momentum:

$$\hat{\mathbf{L}} = \sum_{k,n} C_{kn} [\hat{\mathbf{r}}_k \times \hat{\mathbf{p}}_n] = -i\hbar \sum_{k=1}^2 [\mathbf{r}_k \times \nabla_k]. \quad (44)$$

For the two-particle system, the coefficients C_{kn} are as follows:

$$C_{11} = \left(1 - \frac{m_1}{M}\varepsilon_1\right) (1 - \varepsilon_1)^{-1}, \quad (45)$$

$$C_{12} = -\frac{m_1}{M}\varepsilon_1(1 - \varepsilon_1)^{-1}, \quad (46)$$

$$C_{21} = -\frac{m_2}{M}\varepsilon_1(1 - \varepsilon_1)^{-1}, \quad (47)$$

$$C_{22} = \left(1 - \frac{m_2}{M}\varepsilon_1\right) (1 - \varepsilon_1)^{-1}. \quad (48)$$

It is necessary to emphasize that the parameter of noncommutativity of the operators of coordinates and momenta of different particles ε_1 is the quantum-mechanical average of an operator which depends on the modulus of the interaction force between two particles (i.e., on the distance between two particles). Therefore, this operator is independent of motion of the center of mass of the system since the system of equations (23)-(26) admits the separation of motion of the center of mass of the two-particle system as a whole.

Upon the motion of two reference systems relative to one another with constant velocity \mathbf{v} , the operators $\hat{\mathbf{r}}_k$ and $\hat{\mathbf{p}}_k$ are transformed into $\hat{\mathbf{r}}_k - \mathbf{v}t$ and $\hat{\mathbf{p}}_k - m_k\mathbf{v}$. Such a Galilei transformation of the system of particles is described by the operator [2]

$$\hat{G}(\mathbf{v}, t) = \exp \left[i\mathbf{v} \cdot (M\hat{\mathbf{R}} - \hat{\mathbf{P}}_c t) / \hbar \right], \quad (49)$$

where M , $\hat{\mathbf{R}}$, and $\hat{\mathbf{P}}_c$ are the mass, operator of coordinate, and operator of momentum of the center of mass of the two-particle system. It is easy to show that the condition for the Galilei invariance of the equation of motion (23)

$$\hat{G}^{-1}(\mathbf{v}, t) \left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] \hat{G}(\mathbf{v}, t) = \left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] \quad (50)$$

is valid for Hamiltonian (25).

The quantity $\varepsilon_1 m_2 / M$ is the average share of the momentum transferred to the second particle under the measurement of the coordinate of the first. The value of this momentum can be estimated as $|\mathbf{F}_{12}| \Delta t$, where Δt is the duration of measurement of the coordinate of the first particle. Therefore, the operator $\hat{\varepsilon}$ can be presented in the form

$$\hat{\varepsilon}(|\mathbf{F}_{12}|) = \frac{|\mathbf{F}_{12}| \Delta t}{|\mathbf{F}_{12}| \Delta t + P_0} = \frac{|\mathbf{F}_{12}|}{|\mathbf{F}_{12}| + F_0}, \quad (51)$$

where P_0 or F_0 is some constant of the relevant dimensional. For the two-particle system, we can construct the quantity F_0 from two constants μ and \hbar appearing in the problem under study as

$$F_0 = \frac{(\mu c^2)^2}{\hbar c}, \quad (52)$$

i.e., this is the ratio of the energy of rest of the particle with reduced mass μ to its Compton wavelength. Therefore, the parameter of noncommutativity of the operators of coordinates and momenta of different particles can be presented in the form:

$$\varepsilon_{1l} = \left(\int_0^\infty \chi_{1l}^2(r) \frac{|\mathbf{F}_{12}(r)|}{|\mathbf{F}_{12}(r)| + \frac{(\mu c^2)^2}{\hbar c}} dr \right) \left(\int_0^\infty \chi_{1l}^2(r) dr \right)^{-1}. \quad (53)$$

The proposed method of determination of the parameter of noncommutativity of the operators of coordinates and momenta of different particles contains no parameters and therefore substantially differs from the phenomenological method, proposed in [4]. In the latter method, the representation of the operator $\hat{\varepsilon} = 1 - \exp(-\Omega_0 F_{12}^2 (|\mathbf{r}_2 - \mathbf{r}_1|))$ includes the parameter Ω_0 , whose determination is ambiguous.

Now we consider the situation where a two-particle system has N quantum states, each of them is characterized by the wave function Ψ_1, \dots, Ψ_N . Let the energy of every stationary state be denoted by E_1, \dots, E_N , respectively. If we take the parameter of noncommutativity ε to be the same for each state and equal to, for example, the maximum value of

$$\varepsilon = \max \left\{ \frac{\langle \Psi_1 | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi_1 \rangle}{\langle \Psi_1 | \Psi_1 \rangle}, \dots, \frac{\langle \Psi_N | \hat{\varepsilon}(|\mathbf{F}_{12}|) | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle} \right\}, \quad (54)$$

then operators (21)-(22) will be linear. In this case, the principle of superposition is valid for states. The probabilistic interpretation of wave functions is also conserved.

However, such a choice of the parameter of noncommutativity ε is not physically correct because there exist different average values of the modulus of the interaction force between particles in different quantum states, and the parameter of noncommutativity should be generally different in each quantum state. In this case, we have the own self-consistent system of equations of the type of (29)-(30) for each quantum state, i.e., each quantum state possesses the own interaction Hamiltonian. It is possible to reconcile this situation with the principle of superposition and probabilistic interpretation of wave functions analogously to the introduction of spin into the Schrödinger equation by Pauli [6].

We recall that the motion of an electron in the constant homogeneous magnetic field H_z directed along the z axis is described by two equations with regard for the electron spin:

$$\left[\hat{H}_0 + \frac{e\hbar}{2mc} H_z \right] \Psi_1 = E_1 \Psi_1, \quad (55)$$

$$\left[\hat{H}_0 - \frac{e\hbar}{2mc} H_z \right] \Psi_2 = E_2 \Psi_2, \quad (56)$$

where the wave functions Ψ_1 and Ψ_2 describe the states with the projections of the spin onto the z axis $s_z = +\frac{1}{2}$ and $s_z = -\frac{1}{2}$, respectively. Here, \hat{H}_0 stands for the Hamiltonian of the Schrödinger equation for a charged particle in the external electromagnetic field. The full wave function is two-component by the proposition by Pauli and is written in the form of a matrix column:

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}. \quad (57)$$

As a function Ψ^\dagger , we choose the so-called Hermite-conjugate wave function $\Psi^\dagger = (\Psi_1^*, \Psi_2^*)$, whose elements are not only complex conjugate but also transposed. Then the density of probability is given by

$$\Psi^\dagger \Psi = (\Psi_1^*, \Psi_2^*) \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \Psi_1^* \Psi_1 + \Psi_2^* \Psi_2. \quad (58)$$

Consider a system with N quantum states (N can be infinite, and some share of functions corresponds to a discrete spectrum whereas the rest to a continuous one). Similarly to (57), we introduce wave functions, each of them is represented by a matrix with one column and N rows, where Ψ_1, \dots, Ψ_N normed in a proper way describe possible states of the quantum system with the energies E_1, \dots, E_N , respectively:

$$\Psi_1 = \begin{pmatrix} \Psi_1(\mathbf{r}, \mathbf{R}, t) \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}, \quad \Psi_2 = \begin{pmatrix} 0 \\ \Psi_2(\mathbf{r}, \mathbf{R}, t) \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \dots, \quad \Psi_N = \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ \Psi_N(\mathbf{r}, \mathbf{R}, t) \end{pmatrix}. \quad (59)$$

In correspondence with such a construction of state vectors, the quantity Ψ_k is related to that situation where the system has the energy E_k with probability one. Then any quantum state of the two-particle system can be presented as

$$\Psi = \begin{pmatrix} a_1 \Psi_1(\mathbf{r}, \mathbf{R}, t) \\ a_2 \Psi_2(\mathbf{r}, \mathbf{R}, t) \\ \vdots \\ \vdots \\ a_N \Psi_N(\mathbf{r}, \mathbf{R}, t) \end{pmatrix}, \quad (60)$$

where a_k are arbitrary numbers, complex ones in the general case. The requirement that the state vector (57) be unit, i.e., the scalar product of Ψ and the corresponding vector Ψ^\dagger conjugated by Hermite be equal to 1, allows one to interpret $|a_k|^2$ as the probability for the system to be in the state Ψ_k :

$$\int \Psi^\dagger \Psi d\tau = \sum_{k=1}^N |a_k|^2 = 1. \quad (61)$$

Now the wave equation for the fully nonrelativistic two-body problem has the following form:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \Psi_1(\mathbf{r}, \mathbf{R}, t) \\ \Psi_2(\mathbf{r}, \mathbf{R}, t) \\ \vdots \\ \vdots \\ \Psi_N(\mathbf{r}, \mathbf{R}, t) \end{pmatrix} = \begin{pmatrix} \hat{H}(\varepsilon_1) & 0 & 0 & \dots & 0 \\ 0 & \hat{H}(\varepsilon_2) & 0 & \dots & 0 \\ 0 & 0 & \ddots & 0 & \vdots \\ \vdots & \vdots & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & \hat{H}(\varepsilon_N) \end{pmatrix} \begin{pmatrix} \Psi_1(\mathbf{r}, \mathbf{R}, t) \\ \Psi_2(\mathbf{r}, \mathbf{R}, t) \\ \vdots \\ \vdots \\ \Psi_N(\mathbf{r}, \mathbf{R}, t) \end{pmatrix}, \quad (62)$$

where Ψ_k is the normed wave function of the k quantum state and

$$\hat{H}(\varepsilon_k) = \left[-\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} - \frac{\hbar^2(1 - \varepsilon_k)^2}{2\mu} \Delta_{\mathbf{r}} + V(r) \right], \quad (63)$$

$$\varepsilon_k = \langle \Psi_k | \hat{\varepsilon}(|\mathbf{F}_{12}(r)|) | \Psi_k \rangle. \quad (64)$$

We recall that the average value of any function g of the operators $\hat{\mathbf{r}}_1$, $\hat{\mathbf{r}}_2$, $\hat{\mathbf{p}}_1$, and $\hat{\mathbf{p}}_2$ has the following form:

$$\int \Psi^\dagger \hat{\mathbf{g}} \Psi d\tau = \sum_{k=1}^N |a_k|^2 \int \Psi_k^* g[\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \hat{\mathbf{p}}_1(\varepsilon_k), \hat{\mathbf{p}}_2(\varepsilon_k)] \Psi_k d\tau, \quad (65)$$

where the matrix $\hat{\mathbf{g}}$ is diagonal

$$\hat{\mathbf{g}} = \begin{pmatrix} g(\varepsilon_1) & 0 & 0 & \cdots & 0 \\ 0 & g(\varepsilon_2) & 0 & \cdots & 0 \\ 0 & 0 & \ddots & 0 & \vdots \\ \vdots & \vdots & 0 & \ddots & 0 \\ 0 & 0 & \cdots & 0 & g(\varepsilon_N) \end{pmatrix}, \quad (66)$$

and $g(\varepsilon_k) \equiv g[\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \hat{\mathbf{p}}_1(\varepsilon_k), \hat{\mathbf{p}}_2(\varepsilon_k)]$. In (65), the summation is carried on over all discrete states of the system. If a continuous spectrum is available, we perform the summation over the entire discrete spectrum and the corresponding integration over the whole continuous spectrum in (65).

If all ε_k tend to zero, all $\hat{H}(\varepsilon_k)$ become identical and equal to the Hamiltonian of the Schrödinger equation, and all wave functions are the eigenfunctions of this Hamiltonian.

III. DISCRETE SPECTRUM OF A HYDROGENLIKE ATOM WITHIN THE MODEL OF NONCOMMUTING OPERATORS OF COORDINATES AND MOMENTA OF DIFFERENT PARTICLES

Consider the discrete spectrum of a hydrogenlike atom. Let two particles with masses m_1 (electron) and m_2 (atomic nucleus) be bound by the Coulomb potential $V(r) = -Ze^2r^{-1}$, where Z is the charge of the atomic nucleus. The self-consistent system of integro-differential equations for every state with the binding energy E_{nl} (38)-(39) can be written as

$$\left[-\frac{\hbar^2(1 - \varepsilon_{nl})^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) - \frac{Ze^2}{r} \right] \chi_{nl}(r) = E_{nl} \chi_{nl}(r), \quad (67)$$

$$\varepsilon_{nl} = \int_0^\infty \chi_{nl}^2(r) \frac{\frac{Ze^2}{r^2}}{\frac{Ze^2}{r^2} + \frac{(\mu c^2)^2}{\hbar c}} dr, \quad (68)$$

$$\int_0^\infty \chi_{nl}^2(r) dr = 1. \quad (69)$$

Two equations (67) and (69) are the equations for the normed radial functions of a hydrogenlike atom by the Schrödinger theory. Their solutions for bound states are well-known (see, e.g., [7]):

$$\chi_{nl}(r) = N_{nl} r^{l+1} F\left(-n+l+1, 2l+2, \frac{2Zr}{(1-\varepsilon_{nl})^2 n a_0}\right) \exp\left(\frac{-Zr}{(1-\varepsilon_{nl})^2 n a_0}\right), \quad (70)$$

where

$$N_{nl} = \frac{1}{(2l+1)!} \left[\frac{(n+l)!}{2n(n-l-1)!} \right]^{1/2} \left(\frac{2Z}{(1-\varepsilon_{nl})^2 n a_0} \right)^{l+3/2}. \quad (71)$$

Here, $a_0 = \hbar^2/\mu e^2$ is the Bohr radius, and F is a degenerate hypergeometric function. Eigenenergies are

$$E_{nl} = -\frac{\mu c^2 (\alpha Z)^2}{2} \frac{1}{n^2 (1-\varepsilon_{nl})^2}. \quad (72)$$

Here, $\alpha = e^2/\hbar c$ is the fine structure constant, $l = 0, 1, \dots, n-1$, and $n = 1, 2, \dots, \infty$. By substituting $\chi_{nl}(r)$ into Eq. (68), we obtain the nonlinear equation for the determination of ε_{nl} :

$$\eta_{nl} = S_{nl} \int_0^\infty x^{2l+2} \exp(-x) F^2(-n+l+1, 2l+2, x) \left(1 + \frac{4(\alpha Z)^3}{n^2 \eta_{nl}^4 x^2}\right)^{-1} dx, \quad (73)$$

where $\eta_{nl} = 1 - \varepsilon_{nl}$ and $S_{nl} = [(2l+1)!]^{-2} [2n(n-l-1)!]^{-1} [(n+l)!]$.

For a hydrogenlike atom in the ground state, we have:

$$\eta_{10} = \frac{1}{2} \int_0^\infty x^2 \exp(-x) \left(1 + \frac{4(\alpha Z)^3}{\eta_{10}^4 x^2}\right)^{-1} dx. \quad (74)$$

With respect to η_{10} , this equation has solutions if $\alpha Z \leq \alpha Z_c = 0.510107$ (Fig. 1). From two solutions, a solution being closer to unit is suitable. The second should be omitted since it corresponds to the case where the binding energy tends to minus infinity as the interaction constant αZ tends to zero, which is physically unacceptable. For $Z > Z_c$, Eq. (74) has no solutions, which means that the given bound state does not exist.

Fig. 2 displays the binding energy of the ground state of a hydrogenlike atom along with the analogous dependence by the Schrödinger theory. For the sake of comparison, we also present the corresponding solution of the relativistic Klein-Gordon equation for a spinless particle with mass μ in the Coulomb field $V(r) = -Ze^2 r^{-1}$ as

$$E_{nl} = \mu c^2 \left\{ -1 + \left[1 + \alpha^2 Z^2 \left(n-l-0.5 + [(l+0.5)^2 - \alpha^2 Z^2]^{1/2} \right)^{-2} \right]^{-1/2} \right\}. \quad (75)$$

We see that the energy levels are situated below the Schrödinger ones and higher than that computed according to the Klein-Gordon theory. Analogous calculations can be easily

performed for excited states of a hydrogenlike atom (Figs. 3,4). In this case, it turns out that the Schrödinger levels with given n are split into n closely positioned sublevels since the orbital number l can take n values ($l = 0, 1, \dots, n-1$), i.e., the degeneracy is removed. All levels with a given n and different l are situated below the corresponding Schrödinger level.

For a hydrogen atom, the parameter of noncommutativity ε_{nl} is significantly less than 1 ($\varepsilon_{10} = 0.776 \times 10^{-6}$, $\varepsilon_{20} = 0.970 \times 10^{-7}$, $\varepsilon_{21} = 0.324 \times 10^{-7}$). The splitting of the level with $n = 2$ is also very small and is by two orders of magnitude less than that by the Dirac theory for a hydrogen atom.

The parameter of noncommutativity ε of the operators of coordinates and momenta of different particles, presented in Fig. 5, decreases as the quantum numbers n and l increase (for the same Z), i.e., fully nonrelativistic solutions pass into solutions of the Schrödinger equation for large quantum numbers.

A characteristic feature of the fully nonrelativistic equation is the presence of the critical value of the parameter αZ_c for each energy level, which is lacking in the case of the nonrelativistic Schrödinger equation. For example, for levels with $n = 2$, $\alpha Z_c = 1.401098$ for $l = 0$ and $\alpha Z_c = 1.221611$ for $l = 1$.

As the parameter αZ grows, the average distance between particles decreases. For the ground state of a hydrogenlike atom, $\langle |\hat{\mathbf{r}}_2 - \hat{\mathbf{r}}_1| \rangle = 3\hbar(1 - \varepsilon_{10})^2(2\mu\alpha Z)^{-1}$ and takes the minimum value $\langle |\hat{\mathbf{r}}_2 - \hat{\mathbf{r}}_1| \rangle \approx 1.33\hbar/\mu c$ for $Z = Z_c$. With a further increase in the parameter αZ , the self-consistent system of equations (67)-(69) has no solutions in the state with $n = 1$, i.e., the 1S-state cannot exist, and the ground state is the state with $n = 2$ and $l = 0$ (2S-state) if $0.510 < \alpha Z < 0.847$ or $1.222 < \alpha Z \leq 1.401$. In the region $0.847 < \alpha Z \leq 1.222$, the ground state is the state with $n = 2$ and $l = 1$ since $\varepsilon_{21} > \varepsilon_{20}$ (2P-state). Here, we observe the substantial distinction from solutions of the nonrelativistic Schrödinger equation, for which the ground state is, as known, the 1S-state. Solutions of the proposed fully nonrelativistic solution for a hydrogenlike atom are also significantly different from solutions of the Klein-Gordon equation. The latter has the critical value of the interaction constant $\alpha Z_c = 0.5$. Above it, the continuous energy spectrum appears, and there "occurs" the so-called fall to the center.

Now we write down the values of quantum Poisson brackets proposed by Dirac [8]:

$$\{\hat{x}_1, \hat{p}_{1x}\} = 1 - \frac{m_2}{M}\varepsilon_{nl}, \quad (76)$$

$$\{\hat{x}_2, \hat{p}_{2x}\} = 1 - \frac{m_1}{M}\varepsilon_{nl}, \quad (77)$$

$$\{\hat{x}_1, \hat{p}_{2x}\} = \frac{m_2}{M}\varepsilon_{nl}, \quad (78)$$

$$\{\hat{x}_2, \hat{p}_{1x}\} = \frac{m_1}{M}\varepsilon_{nl}, \quad (79)$$

$$\{\hat{x}_1, \hat{x}_2\} = 0, \quad (80)$$

$$\{\hat{p}_{1x}, \hat{p}_{2x}\} = 0. \quad (81)$$

As $\varepsilon_{nl} \rightarrow 0$, these brackets are transformed into the classical Poisson brackets. That is, in this case, we have a complete analogy between classical mechanics and quantum mechanics. Fig. 5 demonstrates that ε significantly differs from zero for systems, whose size is about the Compton wavelengths of particles composing the system. In this case, there is no similar analogy with classical mechanics.

IV. CONCLUSION

The Schrödinger equation for a system of interacting particles is not a strictly nonrelativistic equation because it is grounded on the implicit assumption about finiteness of the interaction propagation velocity. The last means that if the commutator of operators of a coordinate and the corresponding momentum of a free particle is defined as

$$[\hat{x}, \hat{p}_x] = i\hbar, \quad (82)$$

this commutator for a system of coupled particles has the same value $i\hbar$. However, in a nonrelativistic quantum system during measurement of the coordinate of a particle, a whole transferred momentum is distributed over all particles but is not transferred to only the measured one. Therefore, in a system of interacting particles, this commutator should have the form

$$[\hat{x}, \hat{p}_x] = i\hbar\delta, \quad (83)$$

where $0 < \delta \leq 1$.

The rejection of the implicit assumption on finiteness of the propagation velocity of interactions implies the noncommutativity of the operators of coordinates and momenta of different particles. But the operators of coordinates of all particles and operators of momenta of all particles mutually commute that allows one to use these collections as independent variables.

The derived self-consistent system of integro-differential equations allows one to separate the motion of the center of mass of the system, which moves as a free particle.

The properties of solutions of the proposed system of equations significantly differ from those of Schrödinger solutions for systems, whose size is comparable with the Compton wavelength of particles. That is, the consideration of noncommutativity of the operators of coordinates and momenta of different particles is important for the quantum mechanics of atoms with a large charge of nuclei as well as for the phenomena of nuclear physics, for which the size of a system is about the Compton wavelength of particles composing the system.

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FIGURES

FIG. 1. Dependence of the right-hand side of (74) on η for various values of the parameter αZ .

FIG. 2. Binding energy E_{10} of the ground state of a hydrogenlike atom (72) vs the parameter αZ . The upper dotted line corresponds to the Schrödinger theory, $E_S = -\mu c^2(\alpha Z)^2/2$, and the lower dotted line to the corresponding solution of the Klein-Gordon equation (75).

FIG. 3. Binding energy E_{20} of a hydrogenlike atom (72) vs the parameter αZ . The upper dotted line corresponds to the Schrödinger theory, $E_S = -\mu c^2(\alpha Z)^2/8$, and the lower dotted line to the corresponding solution of the Klein-Gordon equation (75).

FIG. 4. Binding energy E_{21} of a hydrogenlike atom (72) vs the parameter αZ . The upper dotted line corresponds to the Schrödinger theory, $E_S = -\mu c^2(\alpha Z)^2/8$, and the lower dotted line to the corresponding solution of the Klein-Gordon equation (75).

FIG. 5. Dependence of the parameter of noncommutativity of operators ε for the lowest states of a hydrogenlike atom vs the interaction constant αZ .









